pK_a Calculations of Aliphatic Amines, Diamines, and Aminoamides via Density Functional Theory with a Poisson-Boltzmann Continuum Solvent Model

By

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Supporting Information Available: Cartesian coordinates and energies (Hartrees) for the lowest energy forms of the studied neutral and protonated aliphatic diamines and aminoamides obtained at B3LYP/6-31++G** level with and without the effect of the solvent, and a Table comparing calculated (B3LYP/aug-cc-pVTZ(-f)) and experimental gas phase proton affinities, basicities, and solvation free energies of aliphatic amines.

11(g) B3LYP/6-31++G** T.E. = -190.54521365227 a.u.

C1	-3.7519567787	3.5248785552	0.2409479010
H2	-4.5175620587	3.0785516422	-0.4222379103
H3	-4.4593838342	5.4263885351	0.4271254250
C4	-4.1083375680	3.1840957404	1.6874063803
H5	-4.0546850833	2.0917103310	1.8252426189
H6	-3.3607841381	3.6411821068	2.3445440410
N7	-5.4195830280	3.7549959564	2.0335231673
H8	-5.5632806716	3.7758371505	3.0384107354
H9	-6.1752583305	3.2065650790	1.6301093942
H10	-2.7965049842	3.0484477102	-0.0105675137
N11	-3.6128020744	4.9735777326	0.0898813288
H12	-3.4763936565	5.2364872880	-0.8815760598

11(aq) B3LYP/6-31++G** T.E. = -190.56102190098 a.u.

C1	-.4279463894	-.4750300018	.4199098643
H2	-1.0845653532	.1131001335	1.0729547314
H3	.2274875384	-1.0694606811	1.0721123073
C4	.4279463894	.4750300018	-.4199098643
H5	1.0845653532	-.1131001335	-1.0729547314
H6	-.2274875384	1.0694606811	-1.0721123073
H7	-.7061660737	-1.9874743591	-.9581874135
H8	-1.9261246442	-1.8632429836	.1222017792
N9	-1.2737572020	-1.3182644209	-.4393646151
N10	1.2737572020	1.3182644209	.4393646151
H11	.7061660737	1.9874743591	.9581874135
H12	1.9261246442	1.8632429836	-.1222017792

11H+(g) B3LYP/6-31++G** T.E. = -190.92137047357 a.u.

C1	-3.6159968042	3.4602493586	0.2648313328
H2	-4.2539143204	3.0238536246	-0.5069758583
N3	-3.7506706774	4.9621673272	0.1341720912
H4	-2.9518431684	5.4667701617	0.5282526805
H5	-3.8897212932	5.2827295495	-0.8265716834
H6	-4.6066012394	5.1525723286	0.7309528089
C7	-4.1217471520	3.1063027367	1.6779465680
H8	-4.2720556756	2.0234135123	1.7379280761
H9	-3.3646084889	3.3725917541	2.4221518458
N10	-5.3325186477	3.9029841379	1.9302713842
H11	-5.4456455021	4.1315989710	2.9136670753
H12	-6.1808002962	3.4259307533	1.6327742103
H13	-2.5819499033	3.1628800024	0.0872207895

11H+(aq) B3LYP/6-31++G** T.E. = -191.03179053404 a.u.

C1	-3.7547399217	3.5338876820	0.2510197712
H2	-4.5356410865	3.1995072988	-0.4370215763

N3	-3.5834624120	5.0104048976	0.0257725923
H4	-2.7980466137	5.3927253185	0.5610707210
H5	-3.3989831359	5.2155422722	-0.9602881082
H6	-4.4211535297	5.5353920637	0.2934626252
C7	-4.1050690687	3.2058270607	1.6977157503
H8	-4.0124420092	2.1174010316	1.8080709735
H9	-3.3643017065	3.6555514449	2.3675152999
N10	-5.4359516865	3.7111100718	2.0650004438
H11	-5.5610823974	3.6604143382	3.0746601203
H12	-6.1644288046	3.1244641252	1.6603150198
H13	-2.8115749168	3.0616724798	-0.0280686481

11H22+(g) B3LYP/6-31++G** T.E. = -191.11214317859 a.u.

N1	-2.2353290904	1.5638120207	-0.0627605819
H2	-2.8506832383	1.1593579139	-0.7834167052
H3	-2.5066590443	1.1534238784	0.8425309296
C4	-2.2456450781	3.0824352168	-0.0550041278
H5	-1.5188540686	3.3904586912	0.7021651470
H6	-1.8870580580	3.3968737484	-1.0393584885
C7	-3.6582208872	3.6212967420	0.2456645930
H8	-4.3849151063	3.3136807855	-0.5117530383
H9	-4.0169494358	3.3064505388	1.2298249366
N10	-3.6683801543	5.1399088804	0.2541376464
H11	-3.0531370059	5.5439469495	0.9751347131
H12	-3.3968269925	5.5507513423	-0.6508910317
H13	-4.6196162827	5.4839259318	0.4566490073
H14	-1.2840950196	1.2198207013	-0.2652654088

11H22+(aq) B3LYP/6-31++G** T.E. = -191.49594333509 a.u.

N1	-2.2439078124	1.5906583063	-0.0602573913
H2	-2.8655221930	1.1971224906	-0.7743844179
H3	-2.5205885466	1.1926707983	0.8432888357
C4	-2.2505378427	3.0892063347	-0.0540327084
H5	-1.5331099636	3.4077386475	0.7054777373
H6	-1.9008495637	3.4129279816	-1.0368312931
C7	-3.6536132424	3.6144226890	0.2432417317
H8	-4.3708565264	3.2978585951	-0.5172900319
H9	-4.0041890315	3.2886964830	1.2250835564
N10	-3.6595434364	5.1131878012	0.2527928260
H11	-3.0379028602	5.5045549270	0.9680932730
H12	-3.3825521119	5.5131788392	-0.6498538408
H13	-4.6011339320	5.4645781885	0.4549911330
H14	-1.3022793362	1.2388494992	-0.2617676225

12(g) B3LYP/6-31++G** T.E. = -229.86202517009 a.u.

C1	-2.1782485405	3.0683827992	-0.0956327738

H2	-1.4563662036	3.4619067935	0.6334315436
C3	-2.2586599504	1.5413580583	0.0248526329
H4	-2.9731424539	1.1603238744	-0.7162111289
H5	-2.6659707254	1.2882099237	1.0185548871
H6	-0.2763286320	1.1635430182	0.4573676104
C7	-1.8066542453	3.5970382508	-1.4869117628
H8	-2.0091715448	4.6747469451	-1.5166286633
H9	-3.1611161059	3.4713478327	0.1827682298
H10	-0.1702079641	2.4061052935	-1.7772858732
H11	-2.4786694117	3.1279952066	-2.2298943238
H12	-1.0500016504	-0.1189058185	-0.2022198689
N13	-0.9626689651	0.8931362657	-0.2443118396
N14	-0.3818150374	3.4022299421	-1.7793770941
H15	-0.1440955331	3.7821477448	-2.6916374706

12(aq) B3LYP/6-31++G** T.E. = -229.87738195264 a.u.

C1	-3.6294911611	3.6378601590	0.3943755190
H2	-4.3679605622	3.0774355513	-0.1974997596
H3	-3.8729201878	3.4625176431	1.4488222282
H4	-3.5200585132	5.2698744453	-0.8532512832
C5	-2.2331344596	3.0948920237	0.0920080166
H6	-1.5371452063	3.3494242413	0.9029992403
H7	-1.8452713693	3.5688276761	-0.8214630569
C8	-2.2223065739	1.5843726116	-0.1243075376
H9	-2.8922554776	1.3299582788	-0.9555541599
H10	-2.6199286578	1.0660359166	0.7567591611
N11	-0.8866979955	1.0416470497	-0.4212242773
H12	-0.2570203776	1.2109677158	0.3624018225
H13	-0.4841110425	1.5348936107	-1.2182192823
H14	-4.6286531661	5.4474227474	0.3349994729
N15	-3.6980764961	5.0850469122	0.1336696241

12H+(g) B3LYP/6-31++G** T.E. = -230.25011928276 a.u.

C1	-2.2454360574	3.0911502413	-0.0667978217
H2	-1.5989656386	3.5069032593	0.7181726310
C3	-2.2384232890	1.5554348461	-0.0096528886
H4	-2.9170309930	1.1564483741	-0.7705557259
H5	-2.6053304267	1.2132992962	0.9635206378
H6	-0.3057832647	1.0032776987	0.5429514149
C7	-1.8333966454	3.6428827990	-1.4341839942
H8	-1.8901925440	4.7320308089	-1.4828832842
H9	-3.2556852888	3.4537329941	0.1494773369
N10	-0.4079125802	3.2151511701	-1.7408408766
H11	-0.3344715443	2.2002953769	-1.3263931356
H12	0.2737508879	3.8105838340	-1.2639345422
H13	-0.1948957902	3.2394470175	-2.7405227459

H14	-2.4575786151	3.2274156643	-2.2297619212
H15	-0.9165144254	0.0676716432	-0.6401525341
N16	-0.8718990649	1.0284280700	-0.3050279499

12H+(aq) B3LYP/6-31++G** T.E. = -230.34993195958 a.u.

C1	-2.2083674944	3.0761238912	-0.0699843888
H2	-1.5322799270	3.4668025993	0.7029427289
C3	-2.2516058685	1.5431936027	-0.0127331915
H4	-2.9259108133	1.1726733561	-0.7933346359
H5	-2.6768734470	1.2319766574	0.9512758242
H6	-0.3462260274	1.0206191860	0.5922614189
C7	-1.8234074704	3.6380339095	-1.4391026713
H8	-1.9219290478	4.7248606103	-1.4751153674
H9	-3.2065277133	3.4608094095	0.1700801850
N10	-0.3943857389	3.3014266376	-1.7829719588
H11	-0.2269868765	2.3080813431	-1.5103038255
H12	0.2680225797	3.8895610641	-1.2695010834
H13	-0.1978499426	3.4277236881	-2.7793087908
H14	-2.4449901779	3.2057455749	-2.2278372409
H15	-1.0038254061	-0.0457285882	-0.4433887266
N16	-0.9135428419	0.9515367424	-0.2531567909

12H22+(g) B3LYP/6-31++G** T.E. = -230.46416757867 a.u.

C1	-3.6553808045	3.6198982974	0.2459010223
H2	-4.3756554078	3.2990871382	-0.5108236984
H3	-4.0094600297	3.2927103169	1.2266699265
N4	-3.7159089897	5.1410999747	0.2642852530
H5	-3.1066865526	5.5514893594	0.9842552375
H6	-3.4501354432	5.5574810715	-0.6379042233
C7	-2.2352337029	3.1076389718	-0.0552032900
H8	-1.5370204329	3.4785088255	0.7061472787
H9	-1.9033069859	3.4842217149	-1.0312680160
C10	-2.2309633402	1.5682142693	-0.0611642398
H11	-2.8904736194	1.1598004251	-0.8309494323
H12	-2.5245705130	1.1541074742	0.9066306532
N13	-0.8462219554	1.0073190984	-0.3546227131
H14	-0.1491135565	1.2908265259	0.3465049373
H15	-0.4911581248	1.2951984763	-1.2760243921
H16	-4.6731405173	5.4613489919	0.4681228485
H17	-0.8667221574	-0.0222332945	-0.3530778986

12H22+(aq) B3LYP/6-31++G** T.E. = -230.81918286187 a.u.

C1	-3.6563527833	3.6161674619	0.2419058028
H2	-4.3734958935	3.2989543659	-0.5187132235
H3	-4.0099676454	3.2845943900	1.2208388192
N4	-3.6916040899	5.1188176984	0.2624789434

H5	-3.0753870544	5.5107236297	0.9810539124
H6	-3.4106280808	5.5255567135	-0.6350597544
C7	-2.2483440430	3.0983688528	-0.0562058203
H8	-1.5499358358	3.4721978935	0.7022091997
H9	-1.9170445827	3.4714736369	-1.0328712028
C10	-2.2340776639	1.5691723411	-0.0580006736
H11	-2.8954203083	1.1592959100	-0.8248855225
H12	-2.5246179363	1.1608620989	0.9127518363
N13	-0.8589728439	1.0377101424	-0.3508591541
H14	-0.1709055080	1.3387439478	0.3462330367
H15	-0.5148307166	1.3374408177	-1.2683012389
H16	-4.6365942783	5.4602632394	0.4617988300
H17	-0.8543935036	0.0131668633	-0.3521268689

13(g) B3LYP/6-31++G** T.E. = -269.17807081273 a.u.

C1	-3.6355532024	3.7044093448	0.2453800918
H2	-4.3563264815	3.3427157817	-0.4992543544
H3	-3.9912940168	3.3391625274	1.2174199057
N4	-3.7189689895	5.1669912048	0.2661290800
H5	-3.1030488878	5.5599580176	0.9735213919
H6	-3.4433098297	5.5633029690	-0.6289545689
C7	-2.2514179906	3.1021329561	-0.0502299437
H8	-1.5342701288	3.4707979564	0.6982177747
H9	-1.9001228239	3.4753398290	-1.0237286106
C10	-2.2441210077	1.5673257593	-0.0559074242
H11	-2.9608333006	1.1988009182	-0.8048322362
H12	-2.5961074105	1.1941928483	0.9173699872
C13	-0.8597994362	0.9650117931	-0.3505551068
H14	-0.1398233804	1.3259644861	0.3952161950
H15	-0.5029821392	1.3309934707	-1.3219015872
N16	-0.7767241501	-0.4975655190	-0.3726212642
H17	-1.3898612907	-0.8894759307	-1.0830001323
H18	-1.0562314171	-0.8948140364	0.5208397418

13(aq) B3LYP/6-31++G** T.E. = -269.19601168387 a.u.

C1	-3.6511699701	3.6552170104	0.2463818310
H2	-4.3712317775	3.2949495778	-0.4992938697
H3	-4.0067024844	3.2861593120	1.2168099346
N4	-3.6814000813	5.1261194313	0.2602615363
H5	-3.0221597237	5.4707817552	0.9582087983
H6	-3.3485965998	5.4803063669	-0.6362646631
C7	-2.2676027683	3.0933781626	-0.0505211094
H8	-1.5652777543	3.4779052809	0.7017091354
H9	-1.9333868007	3.4797960895	-1.0232468069
C10	-2.2310204202	1.5732819883	-0.0598385065
H11	-2.9319448847	1.1876925408	-0.8129306011

H12	-2.5660324475	1.1867284732	0.9125483697
C13	-0.8455816068	1.0144939125	-0.3544430255
H14	-0.1268157250	1.3819244057	0.3889748220
H15	-0.4927938743	1.3803356497	-1.3270562758
N16	-0.8090006074	-0.4558797925	-0.3612762760
H17	-1.4660174212	-0.8069731678	-1.0580042607
H18	-1.1392681190	-0.8072432381	0.5373008398

13H+(g) B3LYP/6-31++G** T.E. = -269.57448183153 a.u.

C1	-2.3215177346	1.4916057897	-0.0439730844
H2	-3.0626347606	0.7727551285	0.3216076144
C3	-1.1155053722	0.6750678697	-0.5240573639
H4	-0.5910478016	0.2358842916	0.3318588479
C5	-2.0739187891	2.5147343618	1.0858029254
H6	-3.0465164317	2.8099309417	1.4946185074
H7	-1.5388986936	2.0372347235	1.9191356584
C8	-1.3718656597	3.8198676548	0.7029913320
H9	-1.8318765140	4.2721461952	-0.1802056247
H10	-1.4186183333	4.5437018184	1.5199523164
N11	0.0821189988	3.5960865684	0.3625769958
H12	0.6136810921	3.3275385184	1.1944556337
H13	0.5163551612	4.4426116179	-0.0122815031
H14	0.1361377130	2.7526843386	-0.3932418040
H15	0.7113825635	0.9678585722	-1.4742314380
H16	-1.4638426078	-0.1539176931	-1.1491425129
N17	-0.1279746865	1.5104004470	-1.2698626071
H18	-0.5134865935	1.7764180182	-2.1770948921
H19	-2.7939084319	1.9917640742	-0.9013337244

13H+(aq) B3LYP/6-31++G** T.E. = -269.66891640344 a.u.

C1	-2.3215811553	1.4916295498	-0.0466975859
H2	-3.0687593111	0.7780404714	0.3224286051
C3	-1.1262871978	0.6626427605	-0.5365638547
H4	-0.6091680793	0.2191620031	0.3227897597
C5	-2.0607403781	2.5116639843	1.0824778511
H6	-3.0317343623	2.8028615468	1.5011524313
H7	-1.5121165891	2.0313286337	1.9047930630
C8	-1.3682345907	3.8224390061	0.6986945185
H9	-1.8241590876	4.2607685940	-0.1936838927
H10	-1.4431718589	4.5474546217	1.5123149590
N11	0.0907792307	3.6401062593	0.3974882855
H12	0.6196040110	3.3990473002	1.2398047353
H13	0.5050083605	4.4969162793	0.0225571650
H14	0.1973027963	2.8472700023	-0.3206534687
H15	0.6810435382	0.9065648279	-1.5092341653
H16	-1.5055822897	-0.1703407197	-1.1439997675

N17	-0.1396515161	1.4706786305	-1.2903438873
H18	-0.5323592991	1.7510025729	-2.1899513199
H19	-2.7882829112	2.0004207987	-0.9026113034

13H22+(g) B3LYP/6-31++G** T.E. = -269.80565685616 a.u.

C1	-3.6633531631	3.6390924030	0.2491104466
H2	-4.3900896010	3.3290795499	-0.5056894144
H3	-4.0231740614	3.3260352257	1.2322205576
N4	-3.6959874649	5.1642836470	0.2585600934
H5	-3.0732079553	5.5602140473	0.9738887091
H6	-3.4152367028	5.5629261974	-0.6461848258
C7	-2.2561118650	3.1083266725	-0.0489675854
H8	-1.5527738503	3.4780963657	0.7078867381
H9	-1.9179661167	3.4823292431	-1.0236736846
C10	-2.2393124054	1.5610806745	-0.0563930126
H11	-2.9425987084	1.1914324095	-0.8133512538
H12	-2.5775622375	1.1870095691	0.9182281342
C13	-0.8320689400	1.0303791211	-0.3543790106
H14	-0.1056593506	1.3392768228	0.4011787665
H15	-0.4716733958	1.3446577326	-1.3368778986
N16	-0.7997510439	-0.4947930746	-0.3658991171
H17	-1.4222002516	-0.8896200726	-1.0821026218
H18	-1.0810643641	-0.8946540294	0.5381231867
H19	-4.6431503022	5.5114026464	0.4591009817
H20	0.1474372238	-0.8418367329	-0.5664025783

13H22+(aq) B3LYP/6-31++G** T.E. = -270.13845535513 a.u.

C1	-3.6595698412	3.6389632550	0.2413631490
H2	-4.3799468062	3.3306045533	-0.5200442514
H3	-4.0191016421	3.3103439025	1.2192360576
N4	-3.6833972898	5.1446824075	0.2654041492
H5	-3.0636603536	5.5288574397	0.9847374721
H6	-3.3969786525	5.5492844048	-0.6309982133
C7	-2.2599027857	3.1035979912	-0.0541319280
H8	-1.5592591637	3.4764975001	0.7035881973
H9	-1.9220567001	3.4814399216	-1.0271503855
C10	-2.2398707702	1.5644632340	-0.0618092303
H11	-2.9410210896	1.1899186096	-0.8180651294
H12	-2.5760079061	1.1872882662	0.9122305849
C13	-0.8395487469	1.0310079384	-0.3577895469
H14	-0.1162862923	1.3557348520	0.3939223947
H15	-0.4869800664	1.3458093489	-1.3427836284
N16	-0.8060905813	-0.4745820890	-0.3551953078
H17	-1.4326434481	-0.8759981213	-1.0595587883
H18	-1.0767859893	-0.8653294070	0.5525059441
H19	-4.6248203626	5.4949172877	0.4640481303

H20	0.1355798594	-0.8214130436	-0.5603044377

14(g) B3LYP/6-31++G** T.E. = -269.16297465502 a.u.

C1	-3.8668594807	3.5996824372	0.1921960617
H2	-4.7080070962	3.1564438364	-0.3835540326
N3	-3.7112051078	5.0258046587	-0.0581518819
H4	-4.4653740031	5.5171151277	0.4157075205
C5	-4.0859888333	3.3291001145	1.6789719685
H6	-4.0450837812	2.2393364801	1.8649048701
H7	-3.2672052740	3.7880956570	2.2459065844
N8	-5.3395738481	3.9322353637	2.1373729536
H9	-2.9582560632	3.0792406491	-0.1385491338
C10	-3.6691844491	5.3752561609	-1.4714205103
H11	-3.6084892648	6.4624860307	-1.5794230938
H12	-2.7712456132	4.9459397124	-1.9318945737
H13	-4.5428880252	5.0177039547	-2.0492151623
C14	-5.5407365977	3.8447024426	3.5813378173
H15	-6.5191492344	4.2598092106	3.8413696343
H16	-5.4828379405	2.8155094418	3.9801752784
H17	-4.7780747464	4.4434145206	4.0911263426
H18	-6.1194720737	3.4867229831	1.6581976453

14(aq) B3LYP/6-31++G** T.E. = -269.17070107716 a.u.

C1	-2.2324011617	3.1091296538	-0.0392765659
H2	-1.5663752517	3.4080431635	0.7800925028
H3	-1.8514506034	3.6058190284	-0.9505119718
C4	-3.6527044468	3.6033695086	0.2582508681
H5	-4.3667108318	3.1113359448	-0.4275274478
H6	-3.9365939249	3.2991398752	1.2737189382
C7	-0.8538196917	1.0869400856	-0.3010461508
H8	-0.9253654692	0.0024666610	-0.4313806359
H9	-0.2885891961	1.5004585805	-1.1518600508
H10	-0.2714970338	1.2728416060	0.6087883379
C11	-5.0164598755	5.6256065351	0.5849508911
H12	-5.0037771943	6.7102611599	0.4376978302
H13	-5.8774924031	5.2132943528	0.0351421268
H14	-5.1810021629	5.4386482198	1.6519929717
N15	-2.2001045259	1.6480440940	-0.1521044257
H16	-2.7763819456	1.3607078758	-0.9424983803
N17	-3.7254246773	5.0648392105	0.1758812006
H18	-3.5160516195	5.3571383659	-0.7788038754

14H+(g) B3LYP/6-31++G** T.E. = -269.54825417461 a.u.

C1	-3.6313745876	3.4628081013	0.2551078099
H2	-4.2729280718	3.0073879389	-0.5027370767
N3	-3.7673691515	4.9567021092	0.0908547068

H4	-2.9841709429	5.4261381634	0.5546179459
H5	-4.6211734952	5.1464079401	0.6808165976
C6	-4.1140802626	3.1312277754	1.6807655427
H7	-4.2267509933	2.0429209746	1.7729888933
H8	-3.3571312687	3.4435666762	2.4083910583
N9	-5.3545051107	3.8753142639	1.9351361746
H10	-5.4048057311	4.1480928461	2.9121932426
H11	-2.5980720733	3.1637835856	0.0710796550
C12	-6.5961267905	3.1717686998	1.5571562267
H13	-7.4516972328	3.8054996859	1.7989440030
H14	-6.6135174847	2.9867115505	0.4788832385
H15	-6.7085729645	2.2095806157	2.0738726955
C16	-3.9012793675	5.4693265509	-1.3096765841
H17	-3.9955177276	6.5555862615	-1.2791762643
H18	-3.0182144543	5.1853268092	-1.8832539872
H19	-4.7942109203	5.0318317252	-1.7564359618

14H+(aq) B3LYP/6-31++G** T.E. = -269.64204696812 a.u.

C1	-3.8221293687	3.5595310554	0.1890906883
H2	-4.5834660475	3.2087182651	-0.5128007448
N3	-3.7291469370	5.0511550017	0.0194023202
H4	-2.9353484781	5.4070172708	0.5615016897
H5	-4.5679429213	5.4632087099	0.4488078439
C6	-4.1740601967	3.2191803593	1.6370190694
H7	-4.1523535266	2.1220646930	1.7388091773
H8	-3.3963406146	3.6156308533	2.2989460255
N9	-5.4649567121	3.8009158721	2.0250661536
H10	-5.4466581592	4.0237478056	3.0174389553
H11	-2.8564174448	3.1356086816	-0.0951288120
C12	-6.6207980025	2.9401918028	1.7418766513
H13	-7.5318412306	3.4216471944	2.1085284796
H14	-6.7336823106	2.7980966356	0.6621539070
H15	-6.5424312580	1.9439668411	2.2064610293
C16	-3.5935925191	5.5072013238	-1.3998447667
H17	-3.5175932814	6.5955744847	-1.4025399433
H18	-2.6901761768	5.0623764205	-1.8201006975
H19	-4.4732949073	5.1840106736	-1.9575080383

14H22+(g) B3LYP/6-31++G** T.E. = -269.76444246126 a.u.

C1	-2.2380668204	3.1024223930	-0.0563339982
H2	-1.5223336149	3.4352841958	0.7010864896
H3	-1.8884837124	3.4357636196	-1.0378799571
C4	-3.6649544026	3.6023148763	0.2443671167
H5	-4.3809385116	3.2687090369	-0.5124885490
H6	-4.0140586704	3.2696903491	1.2263245856
C7	-0.7809093540	1.0367882607	-0.3614438234

H8	-0.8476274300	-0.0519560424	-0.3486630315
H9	-0.4683063940	1.3880928313	-1.3449478621
H10	-0.1010864876	1.3862556147	0.4158155408
C11	-5.1216849854	5.6679151795	0.5516837210
H12	-5.0554358341	6.7566604697	0.5367482061
H13	-5.8038950524	5.3168098939	-0.2227384564
H14	-5.4309393543	5.3182237273	1.5368210869
N15	-2.1731991459	1.5916819606	-0.0704675076
H16	-2.8210824851	1.2138360619	-0.7736463937
H17	-2.4855487885	1.2131085856	0.8329144471
N18	-3.7301167181	5.1130526056	0.2572273666
H19	-3.4204253028	5.4907515012	-0.6474365923
H20	-3.0803351397	5.4917945938	0.9581719251

14H22+(aq) B3LYP/6-31++G** T.E. = -270.10695048889 a.u.

C1	-2.2426793002	3.1119604554	-0.0555509461
H2	-1.5362790492	3.4514995476	0.7057787141
H3	-1.9035994282	3.4501061384	-1.0377544073
C4	-3.6610691598	3.5924481689	0.2427591200
H5	-4.3668306996	3.2552462582	-0.5202876272
H6	-4.0014909642	3.2522484060	1.2237528744
C7	-0.8186933459	1.0745382927	-0.3556222743
H8	-0.8780980788	-0.0141940019	-0.3407875532
H9	-0.5108641039	1.4292589441	-1.3397269718
H10	-0.1372591794	1.4324462789	0.4168854868
C11	-5.0843420454	5.6307244808	0.5420300006
H12	-5.0240445656	6.7194189522	0.5280131994
H13	-5.7634932537	5.2738523297	-0.2329239704
H14	-5.3959257330	5.2756782812	1.5248993929
N15	-2.1906151554	1.6133918473	-0.0649187817
H16	-2.8450995116	1.2418754645	-0.7620330437
H17	-2.5048162602	1.2439638060	0.8388808935
N18	-3.7116632758	5.0911079337	0.2559596375
H19	-3.3932113893	5.4623373274	-0.6456859125
H20	-3.0599884016	5.4598021281	0.9570401769

15(g) B3LYP/6-31++G** T.E. = -347.77839306972 a.u.

H1	-6.1096744679	7.7293422038	0.5173773565
C2	-4.2935944747	7.7762875141	1.7414025393
H3	-3.2539993492	7.4637748100	1.5978221413
H4	-4.2931244992	8.8811443240	1.8280572593
H5	-5.1595347591	6.2333846025	0.5508467377
C6	-5.0782091800	7.3242881844	0.5020192546
N7	-4.7843775581	7.1617714087	2.9784313266
N8	-4.4056391522	7.6724901390	-0.7530308635
C9	-3.8171789195	7.3163380053	4.0598955712

H10	-2.8611886917	6.8688964520	3.7713947155
H11	-3.6352697367	8.3763284387	4.3293080478
H12	-4.1790647055	6.7983984924	4.9538556456
C13	-6.0921322023	7.6701886456	3.3823621776
H14	-6.4132713043	7.1633962842	4.2976648239
H15	-6.0832016267	8.7617887791	3.5785847179
H16	-6.8396238140	7.4693061702	2.6113136217
C17	-4.4254233899	9.1066528686	-1.0262611995
H18	-3.9176451981	9.6582751639	-0.2316046066
H19	-3.8946449461	9.3066401778	-1.9622137865
H20	-5.4548361044	9.5083346602	-1.1220015529
C21	-4.9702868084	6.9285662805	-1.8740468647
H22	-4.4131059669	7.1604289446	-2.7873778259
H23	-4.8857734649	5.8535835914	-1.6880215311
H24	-6.0381324565	7.1648798348	-2.0560268661

15(aq) B3LYP/6-31++G** T.E. = -347.78375844631 a.u.

C1	-2.2972512179	3.0693769797	-0.1976448074
H2	-1.4491577983	3.4110844560	0.4039594251
H3	-2.1480737820	3.4710527730	-1.2180758318
C4	-3.6032398083	3.6400954159	0.3809696133
H5	-4.4507354236	3.3044261954	-0.2249326223
H6	-3.7560979739	3.2325318279	1.3985845906
C7	-2.7669228172	5.6880356357	1.4246337035
H8	-2.7745574821	6.7803213873	1.3450653424
H9	-3.0944722939	5.4156774498	2.4457687705
H10	-1.7346549909	5.3525878939	1.2975085337
C11	-3.1320490622	1.0111040733	-1.2222343664
H12	-2.8099052692	1.2745040487	-2.2473754478
H13	-3.1213505103	-0.0801141043	-1.1328583375
H14	-4.1646233407	1.3447775182	-1.0948112219
C15	-0.8976597292	1.0920218802	-0.3309725263
H16	-0.8982236443	-0.0012694342	-0.2562993620
H17	-0.4323565998	1.3661184880	-1.2968310716
H18	-0.2702033775	1.4881760706	0.4741343654
C19	-4.9986980840	5.6193530366	0.5250734637
H20	-4.9958262309	6.7131591427	0.4611366975
H21	-5.6237805089	5.2325960225	-0.2862167002
H22	-5.4674604249	5.3360520463	1.4863116622
N23	-2.2671303695	1.5984363734	-0.1937821615
N24	-3.6295847402	5.1116031711	0.3872475142

15H+(g) B3LYP/6-31++G** T.E. = -348.17317578840 a.u.

C1	-3.6000433357	3.4742769862	0.2920439272
H2	-4.2193047489	3.0125164259	-0.4791865991
N3	-3.7189822927	4.9729417084	0.1167035532

H4	-4.5505199110	5.1578599230	0.7377785806
C5	-4.1119657432	3.1298010635	1.7041627350
H6	-4.2583311116	2.0418647672	1.7737453483
H7	-3.3577246859	3.3975985406	2.4500517398
N8	-5.3342128982	3.9012734350	1.9747057107
H9	-2.5631205012	3.1709901928	0.1337190252
C10	-4.0232964721	5.3895866825	-1.2885429049
H11	-4.1454395963	6.4732489874	-1.3180735077
H12	-3.1980427215	5.0911304090	-1.9376078771
H13	-4.9455236595	4.9063750337	-1.6121966316
C14	-2.5435106695	5.7194500119	0.6722862921
H15	-2.7623283666	6.7876831857	0.6542460099
H16	-2.3649179074	5.4009385239	1.6988748835
H17	-1.6668585457	5.5077616410	0.0577892565
C18	-5.5185371265	4.1883735892	3.4086730410
H19	-6.3924040575	4.8316968980	3.5354968637
H20	-5.6722189740	3.2729848187	3.9998718360
H21	-4.6453552037	4.7160500492	3.8012728166
C22	-6.5381721811	3.2597411415	1.4149222681
H23	-7.3966218385	3.9223190202	1.5465825023
H24	-6.4178677451	3.0742775579	0.3435564934
H25	-6.7570610736	2.2998326362	1.9072101406

15H+(aq) B3LYP/6-31++G** T.E. = -348.25470968650 a.u.

C1	-3.7172976967	3.5538140078	0.2711857930
H2	-4.4170116149	3.1339399414	-0.4547919767
N3	-3.6996131879	5.0505825356	0.0404968785
H4	-4.5304087997	5.4033530674	0.5424900099
C5	-4.1377350909	3.2331859713	1.7070720370
H6	-4.1780965269	2.1345392534	1.8070086932
H7	-3.3692297003	3.5793423519	2.4048013746
N8	-5.4098411916	3.8822096697	2.0537998459
H9	-2.7195226690	3.1666815585	0.0506100274
C10	-3.8400927568	5.3954047727	-1.4132395667
H11	-3.8418597836	6.4819795254	-1.5129064979
H12	-2.9954361067	4.9647596800	-1.9540032080
H13	-4.7788114020	4.9815363418	-1.7834267205
C14	-2.4904029692	5.7167807069	0.6328941297
H15	-2.6001164695	6.7956250340	0.5124692996
H16	-2.4180197985	5.4690134142	1.6917002387
H17	-1.6071285430	5.3600646077	0.0994694631
C18	-5.5524714071	4.0588057672	3.5049804323
H19	-6.4751222626	4.6098469466	3.7157674978
H20	-5.5952011508	3.0962486437	4.0464892326
H21	-4.7107329942	4.6387372305	3.8957527167
C22	-6.5685878116	3.1614283536	1.5091774453

H23	-7.4820269630	3.7268229858	1.7185473035
H24	-6.4843560600	3.0542505907	0.4241375253
H25	-6.6734323092	2.1523204814	1.9473918463

15H22+(g) B3LYP/6-31++G** T.E. = -348.40405923138 a.u

C1	-2.2649526171	3.0672891216	-0.1106999958
H2	-1.4850000914	3.3515448104	0.5980336679
H3	-1.9697592872	3.4076218311	-1.1081800921
C4	-3.6333985102	3.6400557931	0.3036678126
H5	-4.4133296677	3.3559921648	-0.4051647940
H6	-3.9286639266	3.2995112680	1.3010571489
C7	-2.7250412786	5.7549339573	1.3951527185
H8	-2.8422468419	6.8387504645	1.3706500847
H9	-3.0151894913	5.3724964154	2.3749235100
H10	-1.6900370080	5.5019510713	1.1676392920
C11	-3.1730681773	0.9521797716	-1.2018581957
H12	-2.8823605647	1.3339873459	-2.1817073261
H13	-3.0562620902	-0.1316646181	-1.1767153481
H14	-4.2080783962	1.2056660181	-0.9749312976
C15	-0.8277016481	1.0443405247	-0.3504014360
H16	-0.8465977780	-0.0452571025	-0.3162694191
H17	-0.4680068108	1.3840757551	-1.3225050446
H18	-0.1998364210	1.4327003244	0.4521696460
C19	-5.0706375322	5.6628981176	0.5443421057
H20	-5.0517506938	6.7525128735	0.5107670317
H21	-5.6986689599	5.2749352194	-0.2582875403
H22	-5.4300924701	5.3226503268	1.5163561586
N23	-2.2502518258	1.5505587375	-0.1584583957
H24	-2.5582294806	1.1993443803	0.7562215197
N25	-3.6481055238	5.1567962240	0.3518331677
H26	-3.3404081549	5.5082893794	-0.5628403455

15H22+(aq) B3LYP/6-31++G** T.E. = -348.71497947427 a.u.

C1	-2.2620460583	3.0795454144	-0.0990491769
H2	-1.5049566613	3.3554501975	0.6366744409
H3	-1.9465644103	3.4282419652	-1.0865801434
C4	-3.6377610444	3.6310505150	0.2807542626
H5	-4.3936942576	3.3609037455	-0.4586200973
H6	-3.9559565015	3.2753479005	1.2650956023
C7	-2.7168556308	5.7141331027	1.3760532337
H8	-2.8519543251	6.7963130376	1.3831196555
H9	-2.9806317937	5.2894667453	2.3466960192
H10	-1.6848643711	5.4794557081	1.1165395914
C11	-3.1803617323	0.9867199920	-1.1761402953
H12	-2.9166458545	1.4029711741	-2.1506175546
H13	-3.0444751152	-0.0955194498	-1.1739080012

H14	-4.2127852730	1.2229870899	-0.9191122387
C15	-0.8479303836	1.0702898765	-0.3434156737
H16	-0.8653804061	-0.0190151064	-0.2912470896
H17	-0.5022348764	1.4024978626	-1.3238615293
H18	-0.2177544012	1.4778591462	0.4480470462
C19	-5.0500057676	5.6379259778	0.5407008105
H20	-5.0325362963	6.7278209017	0.5020385562
H21	-5.6793520934	5.2404603062	-0.2567481462
H22	-5.3981771514	5.2940098711	1.5161982887
N23	-2.2557503404	1.5699249189	-0.1405355949
H24	-2.5612176630	1.2265186576	0.7781447558
N25	-3.6424332262	5.1398329577	0.3343533361
H26	-3.3358360306	5.4901507584	-0.5813199994

16(g) B3LYP/6-31++G** T.E. = -387.09692758244 a.u

C1	-1.1902621209	2.7868776880	-0.0331386154
H2	-0.2435533237	2.7529912151	0.5183006330
C3	-2.0112279680	1.5112308546	0.2021817502
H4	-2.9599995939	1.6001275299	-0.3416808879
H5	-2.2704017861	1.4440463832	1.2792737648
C6	-0.8906287362	3.0396039468	-1.5147432169
H7	-1.8464184032	3.1928739959	-2.0611325575
H8	-1.7645057313	3.6176932879	0.3941478857
N9	0.0321797450	4.1538633104	-1.7468318076
H10	-0.4351217103	2.1360450674	-1.9308650616
N11	-1.3635880165	0.2786053453	-0.2568803714
C12	0.5086585376	4.1635894883	-3.1253454054
H13	0.9908515368	3.2093829198	-3.3589868845
H14	-0.3035362741	4.3281232519	-3.8621926834
H15	1.2486515754	4.9600302835	-3.2555546125
C16	-0.5364552336	5.4487036179	-1.3895279953
H17	0.2025274748	6.2354246758	-1.5712611143
H18	-1.4471997146	5.6918223001	-1.9746335864
H19	-0.7958433345	5.4772695367	-0.3283734824
C20	-2.3100737381	-0.8301204518	-0.2981158776
H21	-3.1490718648	-0.5798600542	-0.9550101679
H22	-1.8183300579	-1.7217134035	-0.7002164409
H23	-2.7189133572	-1.0864869520	0.7002449296
C24	-0.1910578410	-0.0713198414	0.5379479201
H25	0.2606854462	-0.9849001924	0.1391880926
H26	0.5605729672	0.7201924348	0.4873956060
H27	-0.4363892209	-0.2464221479	1.6052359747

16(aq) B3LYP/6-31++G** T.E. = -387.10182510441 a.u

C1	0.9985064051	-0.7725581427	0.5777222966
H2	0.4341696316	-1.3591820914	1.3137047832

H3	1.6162256828	-0.0542507109	1.1536860712
C4	0.0000000000	0.0000000000	-0.2970555761
H5	0.5209858395	0.7124922307	-0.9472292688
H6	-0.5209858395	-0.7124922307	-0.9472292688
C7	-0.9985064051	0.7725581427	0.5777222966
H8	-1.6162256828	0.0542507109	1.1536860712
H9	-0.4341696316	1.3591820914	1.3137047832
N10	1.8511440627	-1.7158409925	-0.1640171659
N11	-1.8511440627	1.7158409925	-0.1640171659
C12	2.8084225414	-1.0398531992	-1.0465583444
H13	2.2847962666	-0.4302254544	-1.7883472619
H14	3.5080208150	-0.3842487692	-0.4918113947
H15	3.4005662007	-1.7868663128	-1.5864692990
C16	2.5516550386	-2.6192207862	0.7549408129
H17	3.1312518604	-3.3531458489	0.1840488321
H18	3.2474471534	-2.0887273975	1.4333014531
H19	1.8261933801	-3.1637052767	1.3699225416
C20	-2.8084225414	1.0398531992	-1.0465583444
H21	-2.2847962666	0.4302254544	-1.7883472619
H22	-3.5080208150	0.3842487692	-0.4918113947
H23	-3.4005662007	1.7868663128	-1.5864692990
C24	-2.5516550386	2.6192207862	0.7549408129
H25	-3.1312518604	3.3531458489	0.1840488321
H26	-3.2474471534	2.0887273975	1.4333014531
H27	-1.8261933801	3.1637052767	1.3699225416

16H+(g) B3LYP/6-31++G** T.E. = -387.49913888526 a.u.

C1	-2.2499586495	3.0896501995	-0.0430497156
H2	-1.6471871876	3.4940942232	0.7778825474
C3	-2.2312419840	1.5525183605	-0.0378399676
H4	-2.8761159202	1.1875896904	-0.8448434113
H5	-2.6493002389	1.1679166816	0.9038798162
C6	-1.8091071442	3.6804777080	-1.3861126734
H7	-1.8529527745	4.7732099739	-1.3984358291
H8	-3.2735696975	3.4308617874	0.1449010189
N9	-0.3898290919	3.2601413144	-1.7294716149
H10	-0.3321968793	2.2703673196	-1.2861213900
H11	-2.4501070728	3.3058592860	-2.1888401692
N12	-0.8632397952	1.0112521369	-0.2708974805
C13	0.6332420228	4.1349244980	-1.0779588879
H14	1.6229424240	3.7045980593	-1.2371048900
H15	0.5884445095	5.1326797451	-1.5199921064
H16	0.4324511677	4.1983858984	-0.0089123654
C17	-0.1622255241	3.1710183450	-3.2035675145
H18	0.8676430163	2.8617011915	-3.3881802819
H19	-0.8469090578	2.4353867154	-3.6276343255

H20	-0.3408662380	4.1472497700	-3.6598580758
C21	-0.9139298620	-0.3439462550	-0.8567198823
H22	0.1031621755	-0.7032673637	-1.0317508086
H23	-1.4243766337	-1.0568072289	-0.1927390728
H24	-1.4440505368	-0.3189004580	-1.8125292183
C25	-0.0740702059	0.9890888630	0.9783559145
H26	0.9476451701	0.6675521631	0.7614267081
H27	-0.0341366076	1.9848497813	1.4268823806
H28	-0.5086747470	0.2988098183	1.7160703788

16H+(aq) B3LYP/6-31++G** T.E. = -387.57490202004 a.u.

C1	-2.2311573919	3.0818947142	-0.0497337949
H2	-1.6186217093	3.4857931272	0.7647092350
C3	-2.2292212009	1.5451259479	-0.0365281534
H4	-2.8729029417	1.1859495522	-0.8471844973
H5	-2.6608181942	1.1721789841	0.9066933146
C6	-1.8057584080	3.6704714198	-1.3982650234
H7	-1.8650050313	4.7621886334	-1.4125237731
H8	-3.2524686916	3.4291249886	0.1443616964
N9	-0.3794268284	3.2805475568	-1.7507825608
H10	-0.2913091551	2.3020845361	-1.3445757013
H11	-2.4427819307	3.2802488376	-2.1969357069
N12	-0.8716351678	0.9799352535	-0.2525484505
C13	0.6343105913	4.1595105034	-1.0848942060
H14	1.6278110890	3.7417466477	-1.2585835110
H15	0.5669455848	5.1614552017	-1.5146528193
H16	0.4338803282	4.2029188275	-0.0140600459
C17	-0.1551444814	3.2267991941	-3.2289173427
H18	0.8791100832	2.9319365034	-3.4166240876
H19	-0.8370394006	2.4948325014	-3.6648850171
H20	-0.3469254309	4.2150723717	-3.6527339074
C21	-0.9363949445	-0.3776339041	-0.8176673198
H22	0.0785826212	-0.7470726950	-0.9939382227
H23	-1.4509095457	-1.0808700655	-0.1408164159
H24	-1.4710377179	-0.3589400248	-1.7719479995
C25	-0.0839080834	0.9714632414	0.9926043359
H26	0.9349431626	0.6344871618	0.7790725753
H27	-0.0302826254	1.9752946745	1.4220508498
H28	-0.5274175827	0.2988740970	1.7462594494

16H22+(g) B3LYP/6-31++G** T.E. = -387.74854861804 a.u.

C1	-3.5862748924	3.6367472302	0.3578391899
H2	-4.3532367023	3.2574814983	-0.3230365468
H3	-3.8387747152	3.3102778809	1.3704809749
N4	-3.7366268748	5.1479523728	0.3520086102
C5	-2.1921170463	3.1404756548	-0.0677574530

H6	-1.4409793969	3.4338779850	0.6743782589
H7	-1.9158192959	3.5945919991	-1.0261318824
C8	-2.2243110961	1.6060680217	-0.1926009011
H9	-2.8617330191	1.2816945853	-1.0198225262
H10	-2.6048420084	1.1541745828	0.7275887905
N11	-0.8648578460	0.9736162230	-0.4340071414
C12	-2.8390342367	5.8532830543	1.3430114092
H13	-3.0831237007	5.4973403092	2.3449636246
H14	-1.7957953622	5.6506265809	1.1046538981
H15	-3.0251739487	6.9253815862	1.2740242058
C16	-0.2311512910	1.3737874759	-1.7468172057
H17	-0.0741250021	2.4513675085	-1.7671170850
H18	0.7294480926	0.8655144221	-1.8346300723
H19	-0.8913034856	1.0637798589	-2.5581671789
H20	-3.4781443465	5.4840506513	-0.5824476947
H21	-0.2365871630	1.2889795925	0.3134968862
C22	-5.1862358472	5.5419042031	0.5650961420
H23	-5.2626803033	6.6273918870	0.4977995138
H24	-5.7990949850	5.0751032567	-0.2064966281
H25	-5.4946087391	5.2046272484	1.5553962948
C26	-0.9493503519	-0.5365969417	-0.3162151490
H27	0.0525109482	-0.9491115288	-0.4375331695
H28	-1.3440070746	-0.7952240383	0.6667554071
H29	-1.6064361011	-0.9091027268	-1.1029829399

16H22+(aq) B3LYP/6-31++G** T.E. = -388.04002554048 a.u.

C1	-3.5924128503	3.6187191652	0.3833417573
H2	-4.3621593500	3.2321076788	-0.2862516207
H3	-3.8377880381	3.3228982420	1.4054554868
N4	-3.7210512269	5.1300681851	0.3333060469
C5	-2.2069403322	3.1129717412	-0.0440802930
H6	-1.4480557517	3.3998911527	0.6907115811
H7	-1.9400972815	3.5637851462	-1.0054148372
C8	-2.2430055877	1.5832604033	-0.1557767762
H9	-2.8888487625	1.2495834681	-0.9723550631
H10	-2.5978881329	1.1371853995	0.7774085882
N11	-0.8760300002	0.9806226137	-0.4140242769
C12	-2.8285395198	5.8326965535	1.3111940855
H13	-3.0637652187	5.4677608259	2.3104670123
H14	-1.7890903929	5.6355545102	1.0588969544
H15	-3.0227244694	6.9017265459	1.2397646217
C16	-0.2694523047	1.4327600202	-1.7149545601
H17	-0.1068011605	2.5138764575	-1.6787145259
H18	0.6864197496	0.9173768175	-1.8384302981
H19	-0.9525656811	1.1711633652	-2.5311597781
H20	-3.4416310892	5.4314092458	-0.6083090233

H21	-0.2561244479	1.2917779364	0.3417357712
C22	-5.1500146136	5.5476744804	0.5323669557
H23	-5.2057392197	6.6281062046	0.4410897110
H24	-5.7568230575	5.0753062980	-0.2329022480
H25	-5.4730743326	5.2313530816	1.5234870667
C26	-0.9332859544	-0.5240730699	-0.3520934346
H27	0.0763960112	-0.9151864853	-0.4841727466
H28	-1.3273519795	-0.8158172855	0.6235678473
H29	-1.5843980298	-0.8787280744	-1.1529205013

17(g) B3LYP/6-31++G** T.E. = -426.41396971906 a.u.

C1	1.5451341519	-0.2251367287	1.5826164395
H2	0.8943076313	-0.8121287654	0.9217785050
H3	2.0883745916	-0.9422471377	2.2111422687
C4	0.6977784502	0.6855921813	2.4828856917
H5	1.3663747130	1.3157977020	3.0830631301
H6	0.0906004473	1.3627760006	1.8684200785
C7	-0.2403315699	-0.1124990219	3.3953856834
H8	-0.8290611374	-0.7972965945	2.7728138278
H9	0.3620336553	-0.7474470529	4.0800334386
C10	2.5267497892	0.5698910648	0.7143461703
H11	3.2454550324	1.1089227989	1.3683079854
H12	1.9640013334	1.3382370148	0.1702142950
N13	-1.1904086077	0.7131844466	4.1453188031
C14	-2.2362490284	-0.1049461130	4.7491574731
H15	-2.7584644727	-0.6739587060	3.9735967549
H16	-1.8455946571	-0.8224384561	5.4989759519
H17	-2.9675467298	0.5393045917	5.2476988057
C18	-0.5444236888	1.5484316969	5.1521936098
H19	-1.3003930866	2.1502818587	5.6660171711
H20	-0.0013242791	0.9545552501	5.9156762134
H21	0.1656722574	2.2354832525	4.6860414608
C22	3.9097093367	0.6073579400	-1.2610092481
H23	4.3718946069	-0.0170844922	-2.0322805969
H24	3.1864385052	1.2686608209	-1.7483687930
H25	4.7033073514	1.2371091871	-0.8101602704
N26	3.2306391114	-0.2377954242	-0.2851203966
C27	4.1632362677	-1.1894686973	0.3092393300
H28	4.6450822039	-1.7706586344	-0.4830721128
H29	4.9582320540	-0.6944114721	0.9037098350
H30	3.6364385994	-1.8903882832	0.9609839058

17(aq) B3LYP/6-31++G** T.E. = -426.41887431610 a.u.

C1	1.4355344525	-0.2138670366	1.4282139078
H2	0.7398119195	-0.8721164980	0.8931046738
H3	2.1009720195	-0.8635377765	2.0118292720

C4	0.6363090897	0.6883529543	2.3807982989
H5	1.3317084685	1.3455388063	2.9177464579
H6	-0.0278703221	1.3390704349	1.7968880722
C7	-0.2118554909	-0.1235809194	3.3682621839
H8	-0.8392915806	-0.8181982309	2.7964646842
H9	0.4521129656	-0.7460300972	4.0014621624
C10	2.2811567733	0.5974471090	0.4379620063
H11	2.9117053044	1.2909894837	1.0076994969
H12	1.6152589983	1.2214829305	-0.1918691676
N13	3.1774501186	-0.2168756929	-0.4000931348
N14	-1.1126843964	0.6903022438	4.2017635839
C15	-2.0983874595	-0.1544248162	4.8844841775
H16	-2.6728534545	-0.7275786111	4.1487517330
H17	-1.6346665398	-0.8689147921	5.5912143839
H18	-2.7977951645	0.4731854965	5.4480010917
C19	-0.3889633969	1.5154237706	5.1742955431
H20	-1.1025108912	2.1144187472	5.7503216560
H21	0.2046302468	0.9095117267	5.8855790090
H22	0.2896766191	2.2045775628	4.6650363505
C23	2.4492918003	-1.0403346357	-1.3707731192
H24	1.7717458141	-1.7294064216	-0.8600140681
H25	1.8535582225	-0.4332257742	-2.0794137979
H26	3.1597912420	-1.6396207257	-1.9502726677
C27	4.1614628598	0.6270319026	-1.0858285007
H28	4.8560122766	-0.0006250208	-1.6551902519
H29	3.6955674103	1.3445166917	-1.7881200538
H30	4.7414419899	1.1972347405	-0.3521844949

17H+(g) B3LYP/6-31++G** T.E. = -426.82062197683 a.u.

C1	-2.3748418500	1.5248898780	-0.0671803474
H2	-3.1326375664	0.8044144025	0.2598455878
C3	-1.2002917658	0.6951250081	-0.6049765802
H4	-0.7264295170	0.1662397837	0.2299244036
C5	-2.0777511025	2.4548482151	1.1275016596
H6	-3.0349829394	2.7544566585	1.5693217523
H7	-1.5568189248	1.9001142610	1.9176427772
C8	-1.3518980959	3.7675581483	0.8174552335
H9	-1.8575322825	4.2875674094	-0.0013623480
H10	-1.3556596412	4.4314036975	1.6876645921
N11	0.0890267408	3.5985033454	0.3935137379
H12	0.0902473274	2.7563302244	-0.3315130739
H13	-1.5829006863	-0.0750770171	-1.2912787336
N14	-0.1385610406	1.4820276281	-1.2903532727
H15	-2.8488904256	2.0971823421	-0.8742852496
C16	-0.5832748720	1.9444212099	-2.6236159807
H17	-1.4723389937	2.5727807339	-2.5367795586

H18	0.2117876273	2.5310023387	-3.0913387407
H19	-0.8224646251	1.0968257074	-3.2816244341
C20	1.0912131545	0.6722211379	-1.4321729697
H21	1.8671647766	1.2640139336	-1.9249268561
H22	1.4526252473	0.3675032282	-0.4463948527
H23	0.9132278116	-0.2319058368	-2.0315608551
C24	0.5998259765	4.8214518150	-0.2956343227
H25	-0.0113740599	5.0188708884	-1.1773069017
H26	0.5494848584	5.6759808867	0.3834203585
H27	1.6353241423	4.6571168175	-0.5980109675
C28	0.9784575873	3.2279590389	1.5353014287
H29	0.9970352614	4.0427675810	2.2630579879
H30	0.6084864397	2.3211224135	2.0123737683
H31	1.9866267319	3.0518682439	1.1572610877

17H+(aq) B3LYP/6-31++G** T.E. = -426.89383554695 a.u.

C1	-2.3696706933	1.5278321289	-0.0723224410
H2	-3.1327893067	0.8118721917	0.2558756196
C3	-1.2020245009	0.6863459327	-0.6090421455
H4	-0.7270232274	0.1638813956	0.2296185918
C5	-2.0673952429	2.4559687517	1.1222984146
H6	-3.0254812833	2.7523419750	1.5659122895
H7	-1.5407353623	1.8993025623	1.9075711867
C8	-1.3510994418	3.7755831957	0.8175581782
H9	-1.8545033058	4.2944519959	-0.0037187502
H10	-1.3641095670	4.4351451698	1.6904468118
N11	0.0965028433	3.6214443979	0.4063732993
H12	0.1137358656	2.8080932646	-0.3076609157
H13	-1.5963284615	-0.0898442709	-1.2862557524
N14	-0.1437994736	1.4580385279	-1.3079304156
H15	-2.8361804987	2.1055721399	-0.8805265924
C16	-0.5931262306	1.9159185352	-2.6372174435
H17	-1.4817433924	2.5451733697	-2.5489263109
H18	0.2005625491	2.5040517296	-3.1067844315
H19	-0.8349060181	1.0632380235	-3.2929901016
C20	1.0796256259	0.6463868141	-1.4477492358
H21	1.8538703665	1.2336065796	-1.9500910891
H22	1.4454026619	0.3527467917	-0.4597721850
H23	0.8948812353	-0.2659040954	-2.0382930894
C24	0.6040652268	4.8556773322	-0.2699945306
H25	-0.0094778122	5.0571279040	-1.1496117366
H26	0.5432053394	5.6965632780	0.4253424657
H27	1.6416414538	4.6952584673	-0.5682696278
C28	0.9811730185	3.2430255244	1.5531827639
H29	0.9698773153	4.0476374006	2.2910607600
H30	0.6227353421	2.3200860628	2.0074531960

H31	1.9949610798	3.0954117747	1.1788751675

17H22+(g) B3LYP/6-31++G** T.E. = -427.08535418260 a.u.

C1	-3.6579236491	3.6685396003	0.0998653775
H2	-4.3342639977	3.3745747693	-0.7077800610
H3	-4.0796249091	3.3142853711	1.0443591149
N4	-3.7166834088	5.1872363830	0.1655028704
H5	-3.0515707675	5.4887471173	0.8861807565
C6	-2.2454050808	3.1059625105	-0.1058491748
H7	-1.5684523345	3.5156676656	0.6557297923
H8	-1.8536432680	3.4007826095	-1.0848483348
C9	-2.2528603075	1.5619392727	-0.0041654892
H10	-2.9306825635	1.1519072413	-0.7647605472
H11	-2.6432494593	1.2674243206	0.9754903035
C12	-0.8407754783	0.9994422627	-0.2115620561
H13	-0.1620561878	1.2982648548	0.5923365313
H14	-0.4225797330	1.3492325314	-1.1592557379
N15	-0.7808425436	-0.5195175930	-0.2693386603
H16	-1.4515883009	-0.8261611874	-0.9825701595
C17	-1.1727868089	-1.1906229048	1.0257912494
H18	-0.4850243585	-0.8619784300	1.8062941048
H19	-2.1977620240	-0.9264942066	1.2812890608
H20	-1.0962893113	-2.2702458141	0.8930546210
C21	0.5843922975	-0.9892868746	-0.7257873459
H22	1.3231832366	-0.6775681687	0.0135730610
H23	0.5703457719	-2.0766256612	-0.8055735980
H24	0.8073036097	-0.5460002254	-1.6966561839
C25	-5.0850969610	5.6560186262	0.6132988284
H26	-5.3172757761	5.2060763648	1.5789593695
H27	-5.0698948030	6.7427422814	0.7010135294
H28	-5.8177681047	5.3508019572	-0.1348586968
C29	-3.3128011049	5.8650789098	-1.1225958411
H30	-3.9937801400	5.5415964825	-1.9111255817
H31	-3.3893596403	6.9440275335	-0.9847072233
H32	-2.2858507742	5.6013905504	-1.3704922208

17H22+(aq) B3LYP/6-31++G** T.E. = -427.36060195329 a.u.

C1	-3.6540928090	3.6520152988	0.1247957631
H2	-4.3473363436	3.3455336769	-0.6642028202
H3	-4.0450379439	3.3099920366	1.0869334111
N4	-3.7065710230	5.1662073149	0.1756603430
H5	-3.0470085148	5.4736062785	0.8996741038
C6	-2.2484670608	3.1005071643	-0.1087307143
H7	-1.5595577116	3.5212757671	0.6347063074
H8	-1.8804757297	3.3846348205	-1.1003341938
C9	-2.2535215117	1.5654593913	0.0071175652

H10	-2.9424043468	1.1451609040	-0.7364945102
H11	-2.6209388718	1.2802659075	0.9986098939
C12	-0.8477041757	1.0151362709	-0.2279752400
H13	-0.1548756333	1.3177679655	0.5630108826
H14	-0.4563791114	1.3623389715	-1.1881715605
N15	-0.7947143506	-0.4985565309	-0.2868966207
H16	-1.4564530815	-0.8024831433	-1.0103817421
C17	-1.2024219174	-1.1562408569	1.0018268652
H18	-0.5402000217	-0.8039427986	1.7950428854
H19	-2.2380969561	-0.9020832663	1.2245502019
H20	-1.1075682199	-2.2357814745	0.8775831397
C21	0.5693548185	-0.9641011594	-0.7155109477
H22	1.2939465117	-0.6551957825	0.0399295600
H23	0.5506643931	-2.0511917180	-0.8035189303
H24	0.8045388191	-0.5116370976	-1.6798408614
C25	-5.0719005199	5.6343154049	0.5976032047
H26	-5.3115747696	5.1846348133	1.5620513781
H27	-5.0525832574	6.7215732546	0.6827620015
H28	-5.7936607645	5.3239725292	-0.1598808988
C29	-3.2942706153	5.8171341735	-1.1150419315
H30	-3.9513342025	5.4582860267	-1.9098557211
H31	-3.3927389370	6.8972062720	-0.9981252525
H32	-2.2565428636	5.5648045778	-1.3308381078

18(g) B3LYP/6-31++G** T.E. = -264.59268713267 a.u.

C1	-1.7024081593	2.3556012969	-0.0237693160
N2	-0.5446008350	1.7995619648	0.4160506648
O3	-1.7894050287	3.4853160517	-0.4953461821
H4	-0.5578375752	0.8492876550	0.7619073594
H5	0.3155093717	2.3196765495	0.3322996598
C6	-2.9343268906	1.4480256854	0.0806458194
H7	-3.7722131473	2.0895381610	0.3817305772
H8	-3.1476473251	1.1098360157	-0.9393771219
N9	-2.7228212696	0.2731974493	0.9347363308
H10	-3.3130879928	-0.5027269093	0.6536473900
H11	-2.9320920501	0.4781795821	1.9076864076

18(aq) B3LYP/6-31++G** T.E. = -264.61601620326 a.u.

C1	-1.6927952942	2.3326989696	-0.0030259487
N2	-0.5149574549	1.8301844694	0.3930316900
O3	-1.8112198795	3.4930745392	-0.4452200112
H4	-0.4505508647	0.8758057151	0.7243490875
H5	0.3244131518	2.3951246436	0.3196497896
C6	-2.9195907692	1.4321275423	0.0638827823
H7	-3.7627353192	2.0781291246	0.3405618005
H8	-3.1040443705	1.1054041665	-0.9673984772

N9	-2.7562039890	0.2551449866	0.9176231033
H10	-3.4657753850	-0.4393439667	0.6898987124
H11	-2.8990374212	0.5011737510	1.8961920496

18H+(g) B3LYP/6-31++G** T.E. = -264.95228962806 a.u.

C1	-1.6584930674	2.2636063119	0.0235878139
N2	-0.4719032072	1.6545451610	0.0031552223
O3	-1.8423276737	3.4648319668	0.2341563877
H4	-0.3606318549	0.6655717527	-0.1724371498
H5	0.3610070031	2.2063245315	0.1730751243
C6	-2.9174854203	1.3980923839	-0.2383696524
H7	-2.9015970297	0.9441265065	-1.2309777023
H8	-3.0395672415	0.6164235847	0.5137573171
N9	-4.0521819054	2.3793655432	-0.1438235236
H10	-4.7088726912	2.1712688634	0.6122435996
H11	-4.5807858293	2.4761257366	-1.0141077912
H12	-3.5316301598	3.2871694425	0.0673898004

18H+(aq) B3LYP/6-31++G** T.E. = -265.08077948511 a.u.

C1	-1.6554306181	2.2726059492	0.0247131680
N2	-0.4951034269	1.6083728986	-0.0137119072
O3	-1.7459310832	3.4903777824	0.2481261962
H4	-0.4466994692	0.6123570338	-0.1929792888
H5	0.3712359762	2.1091989708	0.1570066425
C6	-2.9227278240	1.4500859498	-0.2247244514
H7	-2.8866189490	0.9831884610	-1.2106449208
H8	-3.0212124817	0.6689555708	0.5311172090
N9	-4.1086872361	2.3583914331	-0.1516667428
H10	-4.7697357239	2.0821804290	0.5791251061
H11	-4.6251886724	2.3996619658	-1.0339075126
H12	-3.7803291488	3.3127569525	0.0649787349

19(g) B3LYP/6-31++G** T.E. = -303.90093664284 a.u.

C1	-1.6754292908	2.3189513704	-0.0498856897
N2	-0.5598438560	1.6349056795	0.3135393927
O3	-1.6619304855	3.4211864506	-0.5887162205
H4	-0.6618158397	0.7235835296	0.7399317406
H5	0.3479683642	2.0321060162	0.1255761425
C6	-2.9947491505	1.5838272660	0.2245908437
H7	-3.7340479638	2.3517840980	0.4987589961
H8	-3.3119531822	1.1618454817	-0.7360599861
H9	-3.5419402009	-0.2307242584	0.9973581331
N10	-2.8748566831	0.5050219806	1.2045004872
C11	-3.0263681614	0.9426374767	2.5945229075
H12	-2.9532946305	0.0769990171	3.2591984434
H13	-2.2159636279	1.6323600688	2.8520381981

H14	-3.9818604026	1.4576669553	2.7898229257

19(aq) B3LYP/6-31++G** T.E. = -303.92117353008 a.u.

C1	-1.6698908101	2.2953253938	-0.0306125084
N2	-0.5417059125	1.6515605759	0.2970667676
O3	-1.6731010508	3.4305506046	-0.5458153249
H4	-0.5907889601	0.7208687929	0.6939568807
H5	0.3600172255	2.0774143614	0.1153334693
C6	-2.9906826845	1.5686454128	0.2124841455
H7	-3.7320254354	2.3418652887	0.4712819559
H8	-3.2921139063	1.1568213049	-0.7589858132
H9	-3.6130929765	-0.2065530881	0.9953008570
N10	-2.8992798161	0.4917299353	1.1906206047
C11	-3.0199362879	0.9557918386	2.5789311852
H12	-2.9480653624	0.1014530519	3.2576013431
H13	-2.1973481624	1.6394882291	2.8144488939
H14	-3.9658239748	1.4843738641	2.7788649112

19H+(g) B3LYP/6-31++G** T.E. = -304.27108870532 a.u.

C1	-1.6637578204	2.2694990726	0.0394560359
N2	-0.4712799841	1.6681106684	-0.0195482659
O3	-1.8448906482	3.4695309648	0.2509043860
H4	-0.3588480499	0.6795568958	-0.1954428967
H5	0.3617519313	2.2251856974	0.1293517422
C6	-2.9174365833	1.3854922577	-0.1673903566
H7	-2.8999474955	0.8610490030	-1.1251058026
H8	-3.0219574429	0.6543017769	0.6376909873
N9	-4.0740290786	2.3435910436	-0.1355210202
H10	-4.7362051223	2.0908116556	0.6014368486
H11	-3.5936355007	3.2408371494	0.1452834940
C12	-4.8042690740	2.5408450371	-1.4348676293
H13	-5.5700717167	3.3029004377	-1.2866709169
H14	-4.0868117288	2.8787986485	-2.1830264475
H15	-5.2612418035	1.5986642574	-1.7379748701

19H+(aq) B3LYP/6-31++G** T.E. = -304.38699992389 a.u.

C1	-1.7130016457	2.2790036888	-0.0141519097
N2	-0.5558395444	1.6521388165	-0.2558074880
O3	-1.8160255522	3.5058872372	0.1400462781
H4	-0.4970803276	0.6480209410	-0.3769429551
H5	0.3055631660	2.1892598724	-0.2720602745
C6	-2.9555102006	1.3984679279	0.1128983369
H7	-2.9914545409	0.6065247677	-0.6379535344
H8	-2.9670780905	0.9464040611	1.1087161114
N9	-4.1768557031	2.2495926640	-0.0161278605
H10	-4.9672770129	1.7764415936	0.4318262822

H11	-4.0195389832	3.1128292077	0.5212653940
C12	-4.5469664363	2.6116869019	-1.4239633934
H13	-5.4357598489	3.2425043901	-1.3822322377
H14	-3.7194011129	3.1573350530	-1.8781250547
H15	-4.7534255080	1.6925792578	-1.9746586676

20(g) B3LYP/6-31++G** T.E. = -343.21182239111 a.u.

C1	-1.6900584537	2.3817824512	-0.0165757662
N2	-0.5780692557	1.6565411618	0.2624720601
O3	-1.6853483077	3.5193422783	-0.4854984667
C4	-3.0135580731	1.6530751831	0.2610727641
H5	-3.7191378220	2.4109129566	0.6338818467
H6	-3.3889010129	1.3190574990	-0.7129588587
H7	-3.5581548996	-0.2162112601	0.8975748653
N8	-2.8786973271	0.4951389182	1.1452140504
C9	-2.9843982024	0.8162900018	2.5705373727
H10	-2.8987346639	-0.1018315479	3.1590140494
H11	-2.1607195718	1.4775051147	2.8589470046
H12	-3.9288497131	1.3195023306	2.8370799637
C13	0.7702500594	2.1398682628	0.0276201254
H14	1.3740610608	2.0676513276	0.9386621796
H15	1.2646083835	1.5715742527	-0.7689921353
H16	0.7045727567	3.1858302157	-0.2763468313
H17	-0.7475396255	0.7267897006	0.6303256880

20(aq) B3LYP/6-31++G** T.E. = -343.22884049060 a.u.

C1	-1.6813691468	2.2808596469	-0.0452707153
N2	-0.5505049050	1.6493238998	0.2864672666
O3	-1.6873047815	3.4118309225	-0.5762399076
C4	-3.0002839680	1.5544049992	0.2133442703
H5	-3.7408900130	2.3316258500	0.4641453664
H6	-3.3091595736	1.1227355277	-0.7470783707
H7	-3.6307099954	-0.1988520559	1.0386258230
N8	-2.9075149773	0.4952144117	1.2127208919
C9	-3.0122845926	0.9852261444	2.5928065405
H10	-2.9807608602	0.1394006148	3.2843809156
H11	-2.1627653862	1.6364917918	2.8221400542
H12	-3.9356619964	1.5556525766	2.7808782421
C13	0.7676936977	2.2338114647	0.0658355475
H14	1.5274747718	1.5127861863	0.3716336764
H15	0.9123625935	2.4798217611	-0.9906885310
H16	0.8905220484	3.1518072144	0.6522451307
H17	-0.6438546638	0.7263492317	0.6960638859

20H+(g) B3LYP/6-31++G** T.E. = -343.58595057339 a.u.

C1	-1.2896892452	1.8850245169	0.0846536039

N2	-0.7388214443	2.5370520712	-0.9394439973
O3	-0.7043493538	1.5121314592	1.1095874099
C4	-2.8007189829	1.5514588411	-0.0162732722
H5	-3.4161109590	2.4378530649	-0.1831759267
H6	-2.9935863235	0.8276120125	-0.8114788698
C7	-4.0184407264	1.7648140555	2.2125088916
H8	-4.1265968889	1.2408333441	3.1627400487
H9	-3.5321379479	2.7269000345	2.3757539920
H10	-4.9927657515	1.9016862242	1.7429653652
N11	-3.1427435401	0.9404563000	1.3126356422
H12	-2.1775511462	0.8437015166	1.7390070015
H13	-3.5422932212	0.0070882195	1.1948659162
C14	0.6843987789	2.8962643205	-1.0010575929
H15	1.1644380766	2.5565739024	-0.0845601465
H16	1.1533450732	2.4111722109	-1.8604094063
H17	0.7897058464	3.9801192556	-1.0886876662
H18	-1.3233848730	2.7922022065	-1.7257175411

20H+(aq) B3LYP/6-31++G** T.E. = -343.69459068821 a.u.

C1	-1.3298717698	1.8209297763	0.0769089295
N2	-0.8541132125	2.6708586594	-0.8367670094
O3	-0.6476894886	1.3431461800	1.0005570324
C4	-2.7880071857	1.3864431840	-0.0798649039
H5	-3.4450880317	2.1978022522	-0.3987940812
H6	-2.8397377041	0.5735178875	-0.8105629432
C7	-3.6612956174	1.8976811289	2.2314311576
H8	-3.9620346731	1.3864392393	3.1469344301
H9	-2.7982954611	2.5359206404	2.4239325836
H10	-4.4899719159	2.4786347333	1.8260119544
N11	-3.2764220440	0.8511105108	1.2279999552
H12	-2.5267307250	0.2709887569	1.6263928816
H13	-4.0708522059	0.2277694996	1.0602582415
C14	0.5455759546	3.0977229895	-0.8510215389
H15	0.7849210620	3.6801155684	0.0445793922
H16	1.2132592515	2.2318493152	-0.8911923598
H17	0.7084732174	3.7166683496	-1.7342944717
H18	-1.4818154108	3.0388405398	-1.5421827021

21(g) B3LYP/6-31++G** T.E. = -382.51354112060 a.u.

C1	-1.6474595136	2.3076135339	0.0758930254
N2	-0.5150647859	1.5441331370	-0.0436147280
O3	-1.5986663630	3.5323216703	0.2040667872
C4	-3.0223462119	1.5952615540	0.0799228315
H5	-3.0832054369	0.8577046335	-0.7278463328
H6	-3.1089739335	1.0374664119	1.0232172573
H7	-3.9940727651	3.2848902657	0.5843239232

N8	-4.1496811344	2.4993207927	-0.0433019298
C9	-4.3445885358	3.0162786810	-1.4006163045
H10	-5.1880127750	3.7129955316	-1.3964173264
H11	-3.4671085342	3.5386864684	-1.8127913099
H12	-4.6056150159	2.1872820448	-2.0690895000
C13	-0.4879102201	0.0900836898	-0.1068904111
H14	-1.4897822236	-0.3325533183	-0.0745804993
H15	-0.0015370489	-0.2455391939	-1.0322703429
H16	0.0797170704	-0.3169935566	0.7404520880
C17	0.7926093512	2.1902735435	-0.0177851701
H18	1.3716550692	1.9016734876	-0.9035968474
H19	0.6514523969	3.2699679331	-0.0096089896
H20	1.3533402609	1.8911507974	0.8772809583

21(aq) B3LYP/6-31++G** T.E. = -382.52987044908 a.u.

C1	-1.6874034448	2.1987938625	-0.0226182560
N2	-0.5016368362	1.5634371845	-0.1491035504
O3	-1.7398021599	3.4435871419	0.0508353734
C4	-2.9744164677	1.3779135406	0.0590988246
H5	-2.9996473932	0.6286029004	-0.7412291405
H6	-2.9597465843	0.8198717242	1.0141845820
N7	-4.1399137656	2.2455684931	-0.0726308664
H8	-4.0221170670	3.0634140644	0.5222114371
C9	-5.4111537976	1.5755412416	0.2066418656
H10	-5.5846840054	0.7826113220	-0.5302354358
H11	-5.4666075930	1.1209811820	1.2094168099
H12	-6.2269674009	2.2990511810	0.1102949348
C13	0.7171245354	2.3822715506	-0.1206594200
H14	1.5719871932	1.7455384259	-0.3533099597
H15	0.6563323354	3.1815706188	-0.8632232409
H16	0.8683293859	2.8384117239	0.8649060492
C17	-0.3405094406	0.1107666308	-0.0726032779
H18	-0.0796229263	-0.2031147168	0.9461415430
H19	-1.2567038405	-0.3947975223	-0.3731632736
H20	0.4580969622	-0.1971493795	-0.7525134677

21H+(g) B3LYP/6-31++G** T.E. = -382.89691881661 a.u.

C1	-1.7358359281	2.1112078538	0.0816472604
N2	-0.5221664439	1.5875878920	-0.0986720638
O3	-2.0057763399	3.3257568330	0.0325736280
C4	-2.9383459296	1.1731949384	0.3807320148
H5	-3.1197659109	0.4573755499	-0.4229244926
H6	-2.8137263408	0.6299795066	1.3193754395
H7	-5.6348595646	0.9516075342	-0.4563323481
H8	-5.9394844920	2.7130528032	-0.3875718362
C9	0.6178280736	2.4751118530	-0.3772151267

H10	1.3714277126	2.3563083069	0.4068767682
H11	1.0588872452	2.2080931479	-1.3420449663
H12	0.2741565840	3.5068834345	-0.4029677163
C13	-0.2103418694	0.1575452001	-0.0343699100
H14	0.2106594285	-0.1714320954	-0.9894216992
H15	0.5267103805	-0.0235802559	0.7539895168
H16	-1.0946972655	-0.4423313086	0.1772591203
N17	-4.1139318399	2.1028054161	0.4895609839
H18	-3.6167321302	3.0397705247	0.3754200598
H19	-4.5225605028	2.0645204892	1.4254051483
C20	-5.1857888477	1.9410814705	-0.5467919498
H21	-4.7333765252	2.0672680380	-1.5308469053

21H+(aq) B3LYP/6-31++G** T.E. = -382.99805200272 a.u.

C1	-1.7876358833	2.1083439885	0.1045647518
N2	-0.5880070938	1.5729586742	-0.1686187797
O3	-2.0323542975	3.3289823877	0.0262887445
C4	-2.9209547898	1.1787843006	0.5635110531
H5	-3.0813847620	0.3347404118	-0.1080302539
H6	-2.7176862478	0.8005174181	1.5680333954
H7	-5.2423484834	1.0909423957	-0.9859758591
H8	-5.7791260340	2.7408331757	-0.5238753969
C9	0.5249215764	2.4376979670	-0.5757589933
H10	1.2774006552	2.4837005823	0.2208700273
H11	0.9899634091	2.0275419507	-1.4776758813
H12	0.1563798186	3.4406733766	-0.7809523292
C13	-0.2441678678	0.1584389630	0.0011575913
H14	0.1450241604	-0.2388400045	-0.9427055329
H15	0.5287834218	0.0592480413	0.7723288951
H16	-1.1067091105	-0.4342380359	0.2983741695
N17	-4.1878930024	1.9728313975	0.6240551581
H18	-3.9455306961	2.9198629570	0.9462029487
H19	-4.8077585919	1.5689504338	1.3303611135
C20	-4.9191624152	2.0880310263	-0.6792805343
H21	-4.2481405545	2.5221094778	-1.4209129704

22(g) B3LYP/6-31++G** T.E. = -343.22037700052 a.u.

C1	0.8238002194	2.5579641967	0.9373359586
H2	1.5786721571	3.0667385194	1.5427949924
C3	2.8336586600	1.1971962421	0.3742643835
N4	1.5334599993	1.5606629953	0.1433675563
O5	3.4986553198	1.6576149095	1.2994219677
H6	1.0595160146	1.1561098015	-0.6511276828
C7	3.4171737341	0.1816931002	-0.5952712885
H8	3.8011276976	-0.6682823257	-0.0248146125
H9	2.7026841717	-0.1806431702	-1.3404197090

H10	4.2662875557	0.6402633707	-1.1104373443
C11	-0.2658294647	1.9509592228	1.8422317801
H12	-0.7846087537	2.7770661132	2.3448873985
H13	0.3730186322	3.2977476372	0.2620382605
H14	0.6432193077	0.2060694625	2.4248066436
H15	0.8715299746	1.4350829377	3.4730152586
N16	0.1856031037	1.0043755191	2.8574514053
H17	-1.0177989981	1.4469200712	1.2205091551

22(aq) B3LYP/6-31++G** T.E. = -343.24375978219 a.u.

C1	0.7633212167	2.6254349429	0.8848334334
H2	1.4708713877	3.2285854589	1.4593630106
C3	2.7392484955	1.2114806058	0.4115226866
N4	1.5260196637	1.6889767226	0.0608867435
O5	3.3514894392	1.6213372132	1.4186918840
H6	1.0644216544	1.2808518385	-0.7432866982
C7	3.3435600880	0.1407209480	-0.4689961348
H8	3.4126657960	-0.7872801475	0.1127979512
H9	2.7647288120	-0.0493608061	-1.3774677161
H10	4.3630889093	0.4411143942	-0.7355283861
C11	-0.1919320277	1.8989218343	1.8397140800
H12	-0.7200649442	2.6491478559	2.4394072629
H13	0.1956068840	3.2919068616	0.2283369105
H14	0.8796833951	0.1818696924	2.2050382297
H15	1.2233062025	1.3865504140	3.2461258588
N16	0.4603170857	0.9400466062	2.7396688790
H17	-0.9564023699	1.3616004036	1.2656332289

22H+(g) B3LYP/6-31++G** T.E. = -343.60615718416 a.u.

C1	0.8363888763	2.7158274065	0.8222966894
H2	1.4809343961	3.4124259755	1.3760124227
C3	2.6063193880	1.0070317553	0.3751458974
N4	1.6554810756	1.8705273554	-0.0541706747
O5	2.7275208219	0.7193316784	1.5877449090
H6	1.6261590618	2.0771860307	-1.0437520786
C7	3.5176128720	0.3904824460	-0.6481809396
H8	3.4963498185	-0.6963190661	-0.5334892201
H9	3.2599183765	0.6553392439	-1.6753772325
H10	4.5409288782	0.7186853710	-0.4398472354
C11	-0.0790108642	1.9613547558	1.7949368591
H12	-0.8592077941	2.6270056862	2.1702130983
H13	0.2003745241	3.3206987610	0.1730451496
H14	1.6488268765	1.0531380927	2.5303278560
H15	0.9274909630	2.1674670391	3.6421493175
H16	-0.5507558839	1.1076046718	1.3040904789
N17	0.7076262802	1.4309949857	2.9673889005

H18	0.2076336771	0.6918965351	3.4664963568

22H+(aq) B3LYP/6-31++G** T.E. = -343.71495357054 a.u.

C1	0.8675613078	2.6866001104	0.8662189053
H2	1.5227622588	3.3350240947	1.4617487892
C3	2.6336957700	1.0181052327	0.3383231642
N4	1.6748020125	1.8749980203	-0.0528404693
O5	2.8237153822	0.7563790257	1.5495801323
H6	1.5693721788	2.0543094876	-1.0447531039
C7	3.4901505592	0.3774712811	-0.7276728899
H8	3.4697632043	-0.7091237165	-0.5945780750
H9	3.1744774767	0.6287906994	-1.7424518933
H10	4.5246080424	0.7096068653	-0.5814301415
C11	-0.0783909900	1.9049634220	1.7876742705
H12	-0.9230598880	2.5349966093	2.0710162474
H13	0.2575655285	3.3383335902	0.2383937186
H14	1.5158044481	1.0625563863	2.8284255164
H15	0.7359464502	2.2530282583	3.7048521437
H16	-0.4584209875	1.0083259184	1.2939274917
N17	0.5911402666	1.4699401300	3.0615897090
H18	0.0356799387	0.7705954733	3.5615186589

23(g) B3LYP/6-31++G** T.E. = -382.52433072400 a.u.

C1	-1.7371585254	1.9102607214	0.0625768758
N2	-1.1894135507	1.6313582288	1.2847737793
O3	-1.0443376317	2.1831530110	-0.9115203988
H4	-1.7561959355	1.5841288274	2.1166745123
C5	-3.2569370399	1.7946157171	-0.0353727548
H6	-3.4660588712	0.9156657260	-0.6576356540
H7	-3.7105694750	1.6063154584	0.9437324932
H8	-3.2928449470	3.2233088961	-1.6171772399
C9	-3.8671106970	3.0312613190	-0.7067940830
H10	-4.9081630499	2.8110452296	-1.0129181687
N11	-3.7983486440	4.2229188640	0.1428518173
C12	-3.8026112116	5.4535270169	-0.6418800391
H13	-2.9625174716	5.4478448113	-1.3417341231
H14	-4.7380154644	5.5949590162	-1.2188457401
H15	-3.6851123356	6.3140297281	0.0246745810
C16	-4.8455688793	4.2475375397	1.1573565852
H17	-4.6992910345	5.1071833114	1.8188190575
H18	-5.8619354446	4.3177833934	0.7199371563
H19	-4.8082869992	3.3445795325	1.7738527142
H20	-0.1941315027	1.7682261085	1.3932201496

23(aq) B3LYP/6-31++G** T.E. = -382.54557396395 a.u.

C1	-1.6688604106	2.2184085477	-0.2656701324

N2	-0.6020649003	1.8093036612	0.4503538597
O3	-1.5728604370	3.1200452019	-1.1186369303
H4	-0.6687565324	1.0747934706	1.1435397171
C5	-2.9903091845	1.5148754484	-0.0066845938
H6	-3.1419490720	0.8103731728	-0.8362422996
H7	-2.9215351147	0.9261612182	0.9116735938
C8	-4.1647055688	2.5063475155	0.0302212788
H9	-3.9981311989	3.2516638543	0.8323316502
H10	-4.1791770622	3.0576765900	-0.9141214400
N11	-5.4667242068	1.8433164978	0.1862066090
C12	-6.5638821994	2.7644650707	-0.1321591285
H13	-6.4554932463	3.1362148886	-1.1563992375
H14	-7.5204069694	2.2352641415	-0.0614471710
H15	-6.6034160249	3.6353533387	0.5489949754
C16	-5.6482730286	1.2781554537	1.5274560757
H17	-6.6161804478	0.7699112986	1.5837623553
H18	-4.8727753760	0.5385994814	1.7426359193
H19	-5.6165179657	2.0519338587	2.3179218857
H20	0.3056415538	2.2286938201	0.2763933194

23H+(g) B3LYP/6-31++G** T.E. = -382.54557396395 a.u.

C1	-1.6428818804	2.3047872458	0.1090617104
N2	-0.5455684016	1.5377229121	0.0328892561
O3	-1.5917115121	3.5446983637	0.0254089300
H4	-0.5770700914	0.5301902241	0.0876069798
C5	-2.9818868118	1.6028207899	0.3434150693
H6	-2.9807396550	0.5922631263	-0.0770468397
H7	-3.1159039811	1.4838270953	1.4253950128
H8	-4.0469227613	2.3840337407	-1.3726654599
C9	-4.1540158950	2.3675577825	-0.2856975614
H10	-5.1116343525	1.9017030650	-0.0400380186
H11	-3.1818923484	4.0837871989	0.1336104244
N12	-4.2029327307	3.8154856229	0.1592391046
C13	-4.7066925997	3.9834603684	1.5594531678
H14	-4.1009638513	3.3871053176	2.2410166493
H15	-4.6252257777	5.0350306680	1.8357594603
H16	-5.7497677211	3.6646866028	1.6061644370
C17	-4.9674100312	4.6677047512	-0.8064956453
H18	-5.9964565262	4.3081587470	-0.8689164336
H19	-4.9549123358	5.6988408382	-0.4521684999
H20	-4.4889280659	4.6109115412	-1.7847556521
H21	0.3562133208	1.9864031288	-0.0717639940

23H+(aq) B3LYP/6-31++G** T.E. = -383.01668054629 a.u.

C1	-1.6132439405	2.2578059915	0.1438612630
N2	-0.5645268414	1.4219149375	0.1460378897

O3	-1.4752392447	3.4970779760	0.0521781200
H4	-0.6763202722	0.4171020950	0.2078776356
C5	-2.9986935665	1.6499886856	0.2987201253
H6	-3.0242458283	0.6425595743	-0.1291951890
H7	-3.1926719307	1.5309788395	1.3717953508
H8	-3.9046089234	2.5295944815	-1.4615656161
C9	-4.1005455442	2.4595713645	-0.3890154850
H10	-5.0715662419	1.9806135850	-0.2431305296
H11	-3.2759107250	4.2806449377	0.0216693502
N12	-4.2285470969	3.8874728473	0.1040037930
C13	-4.6392505903	3.9904667249	1.5434658534
H14	-3.8836636019	3.5213412397	2.1735339880
H15	-4.7177734086	5.0483801421	1.7986578562
H16	-5.6042395479	3.4953034132	1.6698129946
C17	-5.1600510550	4.6710359022	-0.7738954406
H18	-6.1555296790	4.2276323049	-0.7108020766
H19	-5.1819122486	5.7031610642	-0.4199595890
H20	-4.7909796589	4.6348008784	-1.7999843825
H21	0.3773108756	1.7985605046	0.1041785288

Table 1S. Calculated and measured gas phase proton affinities (PA), basicities (GB), and solvation energies of neutral (B) and protonated (BH^+) aliphatic amines (energies in kcal/mol)

	base	PA		GB		ΔG^*_{solv} (B)			ΔG^*_{solv} (BH^+)		
		calc[a]	exp[d]	calc[a]	exp[d]	no aq opt[b]	aq opt[c]	expt[e]	no aq opt[b]	aq opt[c]	expt[f]
1	methylamine	214.53	214.9	206.34	206.6	-3.92	-3.94	-4.56	-78.33	-78.49	-76.4
2	ethylamine	218.24	218.0	210.77	210.0	-4.11	-4.21	-4.5	-73.80	-74.13	-
3	propylamine	219.55	219.4	212.12	211.3	-3.85	-3.87	-4.39	-71.96	-72.28	-71.5
4	isopropylamine	221.08	220.8	213.61	212.5	-3.67	-3.81	-	-70.32	-70.67	-
5	*tert*-butylamine	223.94	223.3	215.83	215.1	-3.71	-3.81	-	-67.01	-67.37	-67.3
6	dimethylamine	221.43	222.2	213.50	214.3	-2.13	-2.23	-4.29	-69.25	-69.47	-68.6
7	diethylamine	228.05	227.6	220.18	219.7	-1.59	-1.65	-4.07	-62.05	-62.30	-63.4
8	dipropylamine	230.38	230.0	222.55	222.1	-1.40	-0.82	-3.66	-58.74	-59.03	-60.5
9	trimethylamine	226.25	226.8	218.79	219.4	-0.71	-0.78	-3.23	-62.14	-62.23	-61.1
10	triethyalamine	234.97	234.7	227.32	227.0	0.30	-0.05	-	-52.85	-53.30	-54.9
mean unsigned error		0.41	±2.0[g]	0.64	±2.0[g]	1.6	1.6	±0.2[g]	1.2	1.1	±3.0[g]

[a]B3LYP/aug-cc-pVTZ(-f) using ZPE and thermal corrections from B3LYP/6-31G**. [b]Single point calculations in the aqueous phase on the B3LYP/aug-cc-pVTZ(-f) gas phase geometries. [c]Geometry reoptimization in the aqueous phase at B3LYP/aug-cc-pVTZ(-f) level. [d]Reference 23. [e]Reference 24. [f]Reference 12. [g]An average uncertainty of experimental data.